Guanidine, (2-benzothiazolyl)-
2582-07-2 | DTXSID20180474

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 208 °C

Global applicability domain: Inside

Local applicability domain index: 3.16e-01

Confidence level: 6.35e-01

Nearest Neighbors from the Training Set

Image not found

Methisazone
Measured: 245
Predicted: 243

Image not found

Imazapyr
Measured: 171
Predicted: 189

Image not found

Anot
Measured: 199
Predicted: 199

Image not found

Sulfacytine
Measured: 167
Predicted: 175